TECHNICAL REPORT N° 29 **December 2000**

SIMPLE SOFTWARE FOR PROTEIN SECONDARY STRUCTURE ESTIMATION

We will talk this time of the probably most popular application of CD spectroscopy: secondary structure estimation of proteins. Despite the many progresses (not so many from hardware, but quite a few from software) the estimation is still an empirical task, requiring much common sense.
CD is fast, it requires little amount of sample, it's also easy to use, but as a stand alone technique is in this field not an absolute tool, as we all know.
While CD power is mainly in the capability to monitor changes in the conformation, it's an invaluable tool also for SSE particularly when properly coupled with NMR and X-ray data.

Many users are looking for *easy* software for the job:

-the commercial Jasco software (JWSSE-480 for the 32 bit Spectra Manager software) is based on least square method, is very easy to use and supported by a proper manual. It's however obviously outdated and not competitive with what you can easily get otherwise. At last it's also rather expensive …., so probably not the best choice*

* *In contrast with this Jasco recently introduced a similar task software for FT/IR, which is clearly far more modern and advanced*

-the Softsec™ software is very popular in US. This is just a conversion program including most popular packages developed by well-known researchers (CCA[1] , CD Estima[2] , Contin[3] , Neural Network[4] , Selcon[5], Varselc[6]). It's very easy to use since it reads directly Jasco formats (from J-500 to current J-800).
Softsec is available from Softwood Company (softwood@aol.com) at a cost of about US$ 600.00

-the DICROPROT software is based on a similar concept. Dr Gilbert Deleage of Lyon has developed it (g.deleage@ibcp.fr) and includes different methods for least square fit as well as Selcom and Varselc. While originally designed for Jobin Yvon data files it can read directly the J-700 16 bit Windows™ ones (for J-800 files a file converter can be obtained freely from Jasco). The package is fully free of charge and you can download from Internet (www.ibcp.fr)

Many more programs can be downloaded from Internet, but these reported are the easy to use ones, operating under Windows™ and requiring no particular skill.
For more do yourself applications it pays to mention also the Curvefitting Analysis program available free from Jasco or the well-known Grams/32 from Galactic Industries (www.galactic.com).

The related literature is absolutely impressive, a few reference articles are listed below[7 8 9] , but it may pay to visit the web (try with www.google.com selecting secondary structure of proteins by CD), you'll find a lot!

But the availability of so many alternative software packages means that there is no absolute tool … so we are going back to what said above: common sense and ancillary techniques must be used with care.

---

[1] Perczel A., Park. K., Fasman G.D. *Anal Biochem.* 203, 1992, 83
[2] Yang J.T.,Wu C.S., Martinez H.M. *Methods Enzymol.* 130, 1986, 208
[3] Provencher S.W., Glokner J. *Biochemistry* 20, 1981, 33
[4] Andrade M.A., Chacon P., Merolo J.J., Moran F. *Protein Eng.* 6, 1993, 383
[5] Sreerama N., Woody R. *Anal. Biochem.* 209, 1993, 321
[6] Manavalan P., Johnson W.C.Jr. *Anal Biochem.* 167, 1987, 76
[7] Greenfield N.J. *Anal Biochem.* 235, 1996, 1
[8] JohnsonW.C.Jr. *Proteins* 7, 1990, 205
[9] Venyaminov S.Y., Vassilenko K.S. *Anal. Biochem.* 222, 1994, 176

E.C.S. European Chirality Services srl via Verdi 6A 23870 Cernusco Lombardone (Lc) Italy
tel/fax (0039)-039-9284368 mob 0349-6907288 e-mail ecssrl@libero.it